LETTER TO THE EDITOR

Calculation of the free-free transitions in the electron-hydrogen scattering S-wave model

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Abstract. The S-wave model of electron-hydrogen scattering is evaluated using the convergent close-coupling method with an emphasis on scattering from excited states including an initial state from the target continuum. Convergence is found for discrete excitations and the elastic free-free transition. The latter is particularly interesting given the corresponding potential matrix elements are divergent.

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The convergent close-coupling (CCC) method has had many successes in the field of electron-impact excitation and ionization of atoms and ions. In this method the total wave function is expanded using N square-integrable states and the close-coupling equations are solved in the form of coupled Lippmann-Schwinger equations for the T-matrix elements (Bray and Stelbovics 1992*a*). The N states are obtained from a truncated orthogonal Laguerre basis, and thus in the limit as N goes to infinity, the states span the entire Hilbert space. The CCC method was tested by Bray and Stelbovics (1992*b*) on the Temkin-Poet (Temkin 1962, Poet 1978) (S-wave) model of electron-hydrogen scattering, where only states of zero orbital angular momentum are retained. The total cross sections for elastic, inelastic and ionization collisions converged, with increasing N, for all projectile energies and agreed with the expected S-wave model solutions, where available.

The success of the method for the S-wave model allowed application to many real electron-atom scattering problems. However, application to ionization processes revealed some fundamental difficulties (Bray and Fursa 1996, Röder *et al* 1997), which have been subsequently best illustrated by returning back to the S-wave model (Bray 1997). Though the total ionization cross section (TICS) was found to be convergent, the underlying singly differential cross section (SDCS) was not necessarily so. The triplet SDCS showed rapid convergence, but the singlet SDCS showed unphysical N-dependent resonances. Furthermore, the SDCS were not found to be symmetric about $E/2$, where E is the total (excess) energy, even though antisymmetry of the total wave function has been ensured explicitly. It was suggested that for both total spin cases the CCC(N) amplitudes should converge (as $N \to \infty$) to a step function, being identically zero past $E/2$ (Bray 1997). The step function model was attacked by Bencze and Chandler (1999) who claimed to have proved (see their Eq.(20)) that the CCC-calculated amplitudes should converge to the true amplitudes as $N \to \infty$, and hence yield symmetric SDCS. This claim was rebutted (Bray 1999*d*) and a number of counterexamples given (Bray 1999*a*, Bray 1999*b*).

Unfortunately, a proof for the step function idea has not been given, only suggestive numerical evidence provided. This has encouraged others to study the problem more closely. Baertschy *et al* (1999) obtained benchmark SDCS using an external complex scaling technique (McCurdy *et al* 1997) that does not require the knowledge of three-body boundary conditions. These were found to be in consistent agreement with the CCC results. Furthermore, Rescigno *et al* (1999) showed how step functions may arise when discretization with short-ranged potentials is used.

To our mind the closest to a proof of the step function idea has been given by Stelbovics (1999). He showed that the close-coupling equations, obtained by using exact target eigenstates to expand the total wave function, have unitarity satisfied with the secondary energy integration ending at $E/2$. This implies a step function in the underlying amplitudes since the coupled equations are formally written with this integration ending at E. Given that the CCC square-integrable target states form an equivalent quadrature rule for the infinite summation over the true target discrete

eigenstates simultaneously with an integration over the true target continuum it is tempting to conclude that for infinite N the CCC equations converge to those obtained using exact target eigenstates, and hence the CCC ionization amplitudes should display a step function behaviour. Furthermore, by comparison with the known SDCS at $E/2$, he observed that the CCC-calculated singlet SDCS appeared to converge to 1/4 the value of the true result, and suggested that the CCC equations appeared to behave like Fourier expansions of the underlying amplitudes. A Fourier expansion of a step function converges to the midpoint of the step height. Therefore, the CCC amplitude at equal energy sharing converges to 1/2 of the step height, and hence the SDCS to 1/4 of the true height.

This interpretation is very exciting because it explains the apparent convergence of the SDCS at $E/2$, even when convergence is lacking at unequal energy-sharing, and how it may be related to the true result. A detailed set of applications to the calculation of equal-energy-sharing fully differential electron-impact ionization of the atomic hydrogen ground state has been given (Bray 1999*c*). Here we examine convergence for scattering from the excited states, and particularly of the free-free transitions. The latter are interesting because it is the free-free V-matrix elements that are responsible for the failure to date of solving the close-coupling equations involving pure atomic (discrete and continuous) eigenstates, and thereby requiring the introduction of a pseudostate approach. Free-free one-electron transitions have been looked at before, see Chrysos and Fumeron (1999) for example. Here, for the first time to the best of our knowledge, free-free transitions involving two electrons are shown to be calculable.

Since we shall only concern ourselves with the S-wave model, momenta will be written as scalars in what follows. The traditional close coupling equations arise upon expanding the total wave function over the complete set of target eigenstates ϕ_n of energy ϵ_n. Though we use a discrete notation, this involves an infinite sum of the bound states $\phi_n(\epsilon_n)$ and an integral $(d\epsilon)$ over the continuum states $\phi(\epsilon)$. The close-coupling equations may be written as coupled Lippmann-Schwinger equations for the T-matrix (Bray and Stelbovics 1992*a*)

$$\langle k_f\phi_f|T_S|\phi_i k_i\rangle = \langle k_f\phi_f|V_S|\phi_i k_i\rangle + \sum\!\!\!\!\!\!\int_n d\epsilon_n \int dk \frac{\langle k_f\phi_f|V_S|\phi_n k\rangle\langle k\phi_n|T_S|\phi_i k_i\rangle}{E+i0-\epsilon_n-k^2/2}. \quad (1)$$

These equations are yet to be solved directly due to the non-existence of the free-free matrix elements $\langle k'\phi(\epsilon'')|V_S|\phi(\epsilon)k\rangle$. We write the cross sections for the discrete transition $i \rightarrow f$ as

$$\sigma_{fi}^{(S)} = \frac{k_f}{k_i}|\langle k_f\phi_f|T_S|\phi_i k_i\rangle|^2, \quad (2)$$

and for an ionization process as

$$\sigma_i^{(S)}(\epsilon) = \frac{k}{\sqrt{2\epsilon}k_i}|\langle k\phi(\epsilon)|T_S|\phi_i k_i\rangle|^2. \quad (3)$$

Then the total cross section $\sigma^{(S)}$, at energies above the ionization threshold ($E > 0$), for scattering from some initial state i is

$$\sigma_i^{(S)} = \sum_{f=1}^{\infty} \sigma_{fi}^{(S)} + \int_0^E \sigma_i^{(S)}(\epsilon) d\epsilon. \tag{4}$$

The continuum integration ending at E comes from the fact that in (1) on the energy shell $\epsilon_n \leq E$. From (4) we see immediately the fundamental problem of the close-coupling equations. Since antisymmetry is explicitly included in the V_S (Bray and Stelbovics 1992*a*) there appears to be a double-counting problem as the energy integration ends at E and not $E/2$. However, as mentioned above, Stelbovics (1999) has shown that there is no contribution to the total cross section from $\langle k\phi(\epsilon)|T_S|\phi_i k_i\rangle$ for $\epsilon > k^2/2$ thereby reducing the integration endpoint to $E/2$ and bringing about consistency with formal ionization theory (Rudge 1968).

In order to solve (1) the CCC method uses N discrete states $\phi_n^{(N)}$, with energies $\epsilon_n^{(N)}$, obtained by diagonalising the target Hamiltonian in an orthogonal Laguerre basis (Bray and Stelbovics 1992*a*). The coupled Lippmann-Schwinger equations then take the form

$$\langle k_f \phi_f^{(N)}|T_S^{(N)}|\phi_i^{(N)} k_i\rangle = \langle k_f \phi_f^{(N)}|V_S^{(N)}|\phi_i^{(N)} k_i\rangle + \sum_{n=1}^{N} \int dk \frac{\langle k_f \phi_f^{(N)}|V_S^{(N)}|\phi_n^{(N)} k\rangle \langle k \phi_n^{(N)}|T_S^{(N)}|\phi_i^{(N)} k_i\rangle}{E + i0 - \epsilon_n^{(N)} - k^2/2}. \tag{5}$$

Using the relation

$$|\phi(\epsilon_f)\rangle = \lim_{N\to\infty} |\phi_f^{(N)}\rangle\langle\phi_f^{(N)}|\phi(\epsilon_f)\rangle, \tag{6}$$

where $\epsilon_f^{(N)} = \epsilon_f$, the total cross section corresponding to (4) becomes

$$\sigma_i^{(SN)} = \sum_{f:\epsilon_f^{(N)}<0} \sigma_{fi}^{(SN)} + \int_0^E \sigma_i^{(SN)}(\epsilon) d\epsilon, \tag{7}$$

where

$$\sigma_i^{(SN)}(\epsilon_f) = \frac{k_f}{\sqrt{2\epsilon_f} k_i} |\langle\phi(\epsilon_f)|\phi_f^{(N)}\rangle\langle k_f \phi_f^{(N)}|T_S^{(N)}|\phi_i^{(N)} k_i\rangle|^2 \tag{8}$$

is the SDCS. For infinite N (7) goes to (4) and hence a step function, with the integration ending effectively at $E/2$.

Similarly, we can write down the relationship between the free-free matrix elements occurring in both (1) and (5). For example,

$$\langle k_f \phi(\epsilon_f)|V_S|\phi(\epsilon_i) k_i\rangle = \lim_{N\to\infty} \langle\phi(\epsilon_f)|\phi_f^{(N)}\rangle\langle k_f \phi_f^{(N)}|V_S^{(N)}|\phi_i^{(N)} k_i\rangle\langle\phi(\epsilon_i)|\phi_i^{(N)}\rangle. \tag{9}$$

Thus, the non-existence of free-free V_S matrix elements in (1) has not been eliminated, and becomes evident with increasing N. However, numerical solutions of (5) have shown good convergence for the T_S matrix elements, at least for excitation of the ground state (Bray and Stelbovics 1992*b*). Here we check for convergence in the case of excited initial states including a free-free transition.

The numerical investigation is performed for the total energy $E = 3$ Ry. The results of three calculations, N=23, 26 and 29, are presented. The states were chosen in such a way so that there was always a state of 1.5 Ry. This way all three calculations contain the matrix elements of the free-free transition corresponding to two 1.5 Ry electrons elastically scattering on a proton. In figure 1 we present the discrete excitation cross sections and the SDCS, evaluated according to (8), for the singlet case. The value ϵ_i is the initial energy of the bound electron when negative, or otherwise the energy of an incident electron.

We begin the discussion of the cross sections for the negative-energy states. Good convergence is seen for the first five states for all four initial states, with elastic scattering being the most dominant. For the higher ($n > 5$) lying discrete states the bigger calculations yield the smaller cross sections, but in all cases the cross sections for the last negative-energy states rise. This is not an indication of divergence from the expected n^{-3} scaling rule, but shows how the least negative-energy states take into account the remaining full infinite discrete spectrum.

Turning our attention to the SDCS from the ground state, for energies less than $E/2$ we observe that there are substantial N-dependent oscillations about the exact result, calculated using the finite difference method (FDM) by Jones and Stelbovics (1999). At $E/2$ the three CCC calculations show convergence to approximately a quarter of the FDM result, as expected.

The SDCS from the 2S and 3S initial states show less oscillation than for the ground state owing to the SDCS at $E/2$ being of relatively small magnitude. Thus, within the same calculations the CCC method is able to obtain SDCS more accurately, over the energy range $[0, E/2]$, from excited states than from the ground state.

Finally, we consider the free-free transitions for the case where the two electrons are both incident at 1.5 Ry. It is seen that the functional form of the SDCS changes as compared to the discrete initial states. Oscillations are very large, but convergence at $E/2$ is evident, and presumably to one quarter of the true value. This suggests that the elastic scattering is the most dominant, which explains the functional form change, and is consistent with the elastic scattering from the presented discrete states being the most dominant of the discrete transitions. It is truly remarkable to see convergence at $E/2$ as the corresponding V_S matrix elements are an order of magnitude greater than the T_S matrix elements and continue to increase with N.

For completeness, in figure 2 we present the cross sections for the triplet case. Here the initial state with two 1.5 Ry electrons is forbidden and so is not presented. All convergence considerations for the discrete excitations apply equally here as in the case of singlet scattering. The SDCS are all free from oscillations owing to the zero cross section at $E/2$, and good agreement is found with the FDM-calculated SDCS available only for the ground state (Jones and Stelbovics 1999).

In summary, the recent work of Stelbovics (1999) has shown that the CCC theory yields convergent ionization scattering amplitudes at equal energy-sharing that are simply a factor of two less than the true amplitudes. Thus, the CCC theory may claim

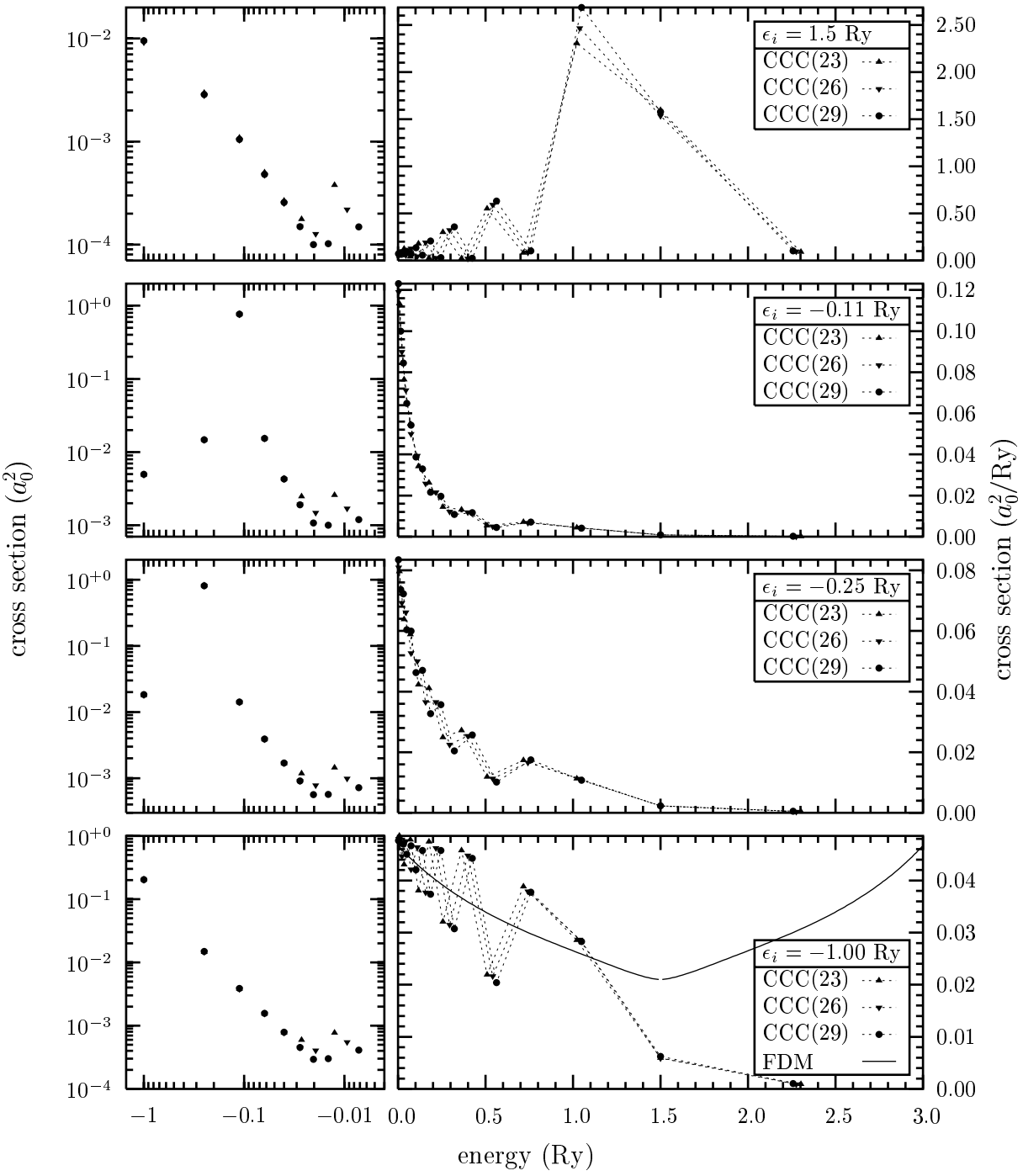

Figure 1. The singlet cross sections arising upon solution of the electron-hydrogen S-wave model at the total energy of 3 Ry for the lowest three discrete (1S, 2S and 3S) initial state, and the $\epsilon_i = 1.5$ Ry state from the target continuum. The present CCC(N) calculations are described in the text. The SDCS calculated by the finite-difference method of Jones and Stelbovics (1999) is denoted by FDM.

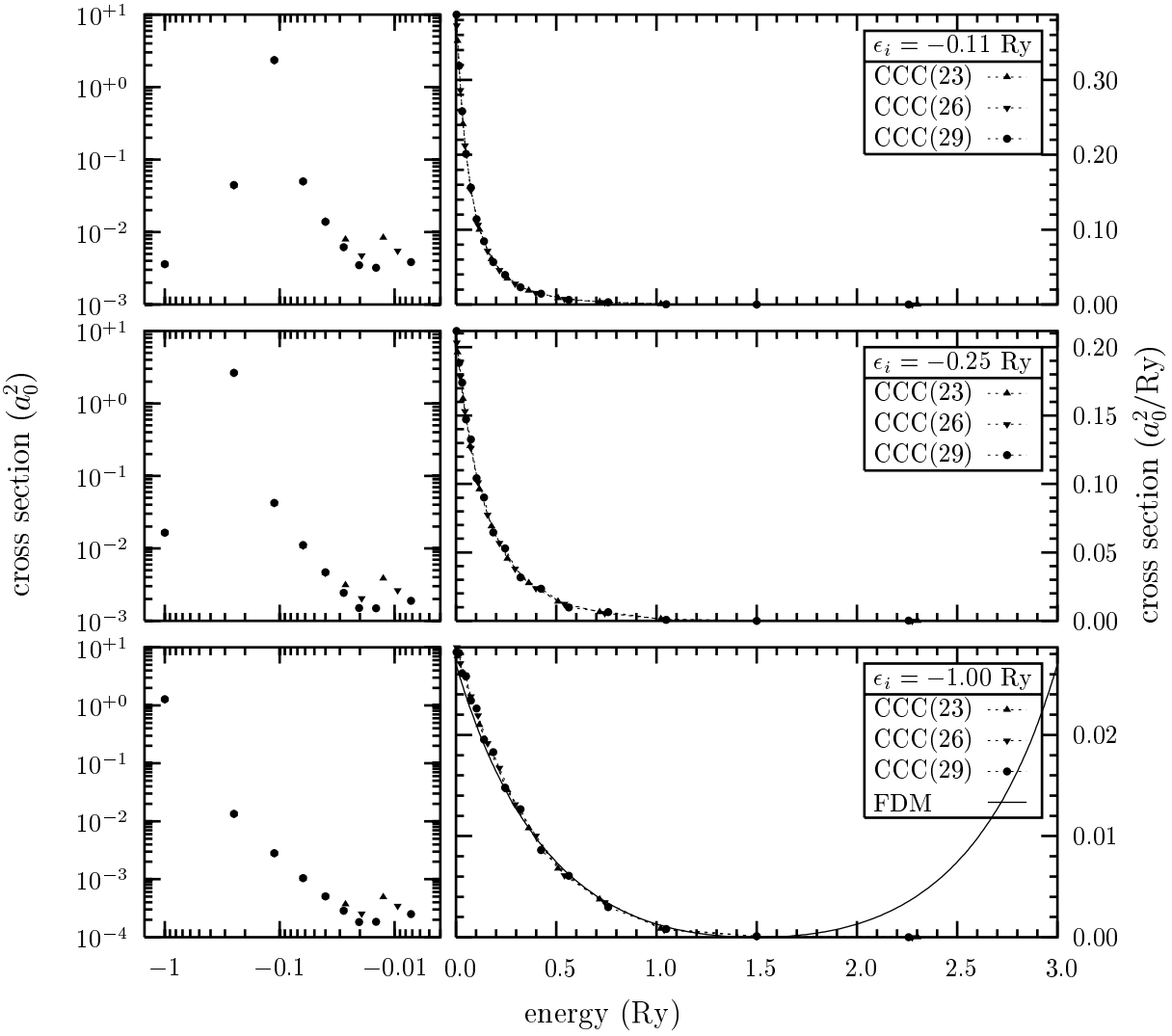

Figure 2. Same as for figure 1 except for the triplet case. No result for scattering from the $\epsilon_i = 1.5$ Ry state is given owing to the Pauli Principle ensuring that such cross sections are zero.

to yield these amplitudes accurately for any initial state, and not only for the S-wave model considered here. We have seen convergence in the model for the elastic free-free transition which corresponds to the real experimental case of equal energy (2e,2e) on a proton. Whereas such processes are yet to be experimentally observed the CCC (e,2e) calculations include such processes as an intermediate step and these may be extracted as convergent cross sections. This is particularly pleasing since the introduction of the L^2 technique in solving the close-coupling equations does not eliminate the divergence of the underlying free-free potential matrix elements, but masks it with a dependence on N. Finally, though Stelbovics (1999) does not claim this, we suggest that his work implies a step function of the underlying amplitudes in forming (4) and hence the CCC-calculated amplitudes used in (7), supporting our initial hypothesis (Bray 1997).

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